RADIAL EQUATIONS OF THE THEORY OF

ATOMIC COLLISIONS [   ]

by

L. A. Vaynshteyn *(USSR)*   *Oct. 1963   23p*

[USSR]

pick up lot. next page

DRAFT TRANSLATION   ST – NPH – 10 053

RADIAL EQUATIONS OF THE THEORY OF
ATOMIC COLLISIONS *

by L. A. Vaynshteyn**

I. INTRODUCTION OF THE POLARIZATION POTENTIAL

1. General System of Radial Equations

The problem of computing the effective cross sections of electron collisions with atoms or ions amounts to the solution of an infinite system of integro-differential equations. In order to conduct real computations taking into account the properties of atom symmetry, it is necessary that these equations be radial equations of the Hartree-Fock multifigurational type. Such equations were obtained in the general case in reference [1]. Naturally, the solution of an infinite system in a general case is impossible; however, the first approximation permits already to account for distortion effects of the incident and scattered wave and exchange. In order to subsequently make these results more precise, it is necessary to add the accounting of atom polarization. A substantial number of works have been lately devoted to this subject (for example [2,5]), but the introduction of the polarization was usually conducted by a special and often somewhat artificial way.

The polarization potential for the elastic scattering was introduced in a general form in [6] on the basis of the formal collision theory. The polarization potential is introduced in the first part of this work for the elastic as well as inelastic scattering on the basis of the standard system of radial equations by way of its solution by the method of consecutive approximations. Some of the approximate representations of this potential are discussed in the second part of the current paper.

For the sake of simplicity reference will be made to neutral atoms in all subsequent considerations; however, all these results are easily generalized to ions by way of the well known modification of boundary conditions.

The effective cross section of the process $a_0 \longrightarrow a$ may be written in the form

$$\sigma_{aa_0} = \sum_{\gamma l} [\sigma_{aa_0}^{+}(\tilde{l l_0}) + \sigma_{aa_0}^{-}(\tilde{l l_0})], \qquad (1a)$$

$$\sigma_{aa_0}^{\pm}(\tilde{l l_0}) = \frac{4k}{k_0} c^{\pm} \sum_{b_\gamma} \frac{2L_T + 1}{2L_0 + 1} |T_{\Gamma \Gamma_0}|^2 \pi a_0^2, \qquad (16)$$

$$c^{\pm} = \frac{2S_T + 1}{2(2S_0 + 1)} = \frac{1}{2}\left(1 \mp \frac{1}{2S_0 + 1}\right), \qquad (1B)$$

where $\Gamma = a\tilde{l}L_T S_T$ is a complete set of quantum numbers of the system from the atom in the state a ($a = \gamma L S$) and the outer electron in the state $k\tilde{l}$, $L_T S_T$ are the system's over-all moments.

The signs $\pm$ correspond to the symmetrical $\left(S_T = S_0 - \frac{1}{2}\right)$ and "antisymmetrical" $\left(S_T = S_0 + \frac{1}{2}\right)$ scattering in correspondence with the symmetry properties of system's radial functions. The initial state is denoted by the index zero. The T-matrix is defined by the asymptotic of outer electrons' wave functions.

The integro-differential equations obtained in the work [1] for these functions, have the form:

$$[L_\Gamma + k^2]F_\Gamma(r) = \sum_{\Gamma' \neq \Gamma}' U_{\Gamma\Gamma'}(r) F_{\Gamma'}(r). \qquad (2)$$

$$F_\Gamma(0) = 0; \quad F_\Gamma \underset{r\to\infty}{\sim} \delta_{\Gamma\Gamma_0} \sin\left(kr - \frac{\bar{l}\pi}{2}\right) + T_{\Gamma\Gamma} \, e^{ikr}. \qquad (3^*)$$

Here L_Γ is the usual Hartree-Fock operator:

$$L_\Gamma = \frac{d^2}{dr^2} - \frac{\bar{l}(\bar{l}+1)}{r^2} - U_\Gamma(r). \qquad (4)$$

The potentials U_Γ and $U_{\Gamma\Gamma_1}$ include the direct as well as the exchange interaction, i.e. they are in the general case the integral operators :

$$U_{\Gamma\Gamma'}F_{\Gamma'} = \sum_{x} \alpha^{x}_{\Gamma\Gamma'} \, y^{x}_{l_1l'}F_{\Gamma'} - \sum_{x} \beta^{x}_{\Gamma\Gamma'} \, y^{x}_{l\tilde{l}'} P_{n'l'}. \qquad (5)$$

$$y^{x}_{l_1l'}(r) = 2 \int_0^\infty \frac{r^x_<}{r^{x+1}_>} P_{nl}(r_1) P_{n'l'}(r_1) \, dr_1. \qquad (5a)$$

$$y^{x}_{l\tilde{l}'}(r) = 2 \int_0^\infty \frac{r^x_<}{r^{x+1}_>} (1 - \delta_{x0}\lambda_{\Gamma\Gamma'} r_>) P_{nl}(r_1) F_{\Gamma'}(r_1) \, dr_1, \qquad (5b)$$

where $r_<$ and $r_>$ are respectively the greater and the lesser of the values of r and r_1, P_{nl} and $P_{n'l'}$ are the radial functions of atom's optical electron.

The diagonal potentials $U_\Gamma = U_{\Gamma c} + U_{\Gamma\Gamma}$, where $U_{\Gamma\Gamma}$ describes the Hartree-Fock interaction with the optical electron, and is determined by the formula (5), and $U_{\Gamma c}$ — the interaction with electrons of atom residuum. To curtail the writing the definition of radial integrals $y_x(r)$ is somewhat different than in the paper [1]. In particular, Rydberg units are used everywhere for energy. The formulae for α, β, γ,, obtained in [1], are given in the Appendix 1.

[N. B.].- If the incident wave is flat, there exist a multitude of values of Γ_0 with the given a_0, but with all kinds of $l_0 L_0 S_0$. This is taken into account when deriving formulae for cross sections. In particular, when computing differential and M- sublevel excitation cross sections, there occurs a wave interference with various l_0. But after the type (1)-formula is written, all partial incident waves may be considered independent when resolving the radial equations (2).

The equation (2), account being taken of boundary conditions (3), may be rewritten in the form of integral equations. Let F, $\bar{\bar{F}}$ be two lineraly independent solutions of a homogenous equation, and let $G(r, r')$ be the Green function :

$$[L+k^2]\bar{F}(r) = 0; \quad [L+k^2]\bar{\bar{F}}(r) = 0, \tag{6}$$

$$[L+k^2]G(r, r') = \delta(r-r'), \tag{7}$$

with $\bar{F}$ and $\bar{\bar{F}}$ satisfying the boundary conditions : $\bar{F}(0) = 0$,

$$\bar{F} \sim e^{i\eta}\sin\left(kr - \frac{l\pi}{2} + \eta\right); \quad \bar{\bar{F}} \sim \frac{1}{k} e^{i\left(kr - \frac{l\pi}{2}\right)} (k^2 > 0), \tag{8a}$$

$$\bar{F} \sim \frac{1}{2} e^{qr}; \quad \bar{\bar{F}} \sim \frac{1}{q} e^{-qr} (k^2 < 0; \quad k = iq). \tag{8b}$$

The Green function is expressed by means of $\bar{F}$ and $\bar{\bar{F}}$:

$$G(r, r') = -\bar{F}(r_<)\bar{\bar{F}}(r_>). \tag{9}$$

Let us introduce besides the integral operator $\hat{G}$:

$$\hat{G}\varphi = \int_0^\infty G(r, r')\varphi(r')\, dr'. \tag{10}$$

Then, the system of integral equations, equivalent to formulae (2) and (3), may be written in the form:

$$F_\Gamma = \bar{\bar{F}}_\Gamma \delta_{\Gamma\Gamma_0} + \hat{G}_\Gamma \sum_{\Gamma'} U_{\Gamma\Gamma'} F_{\Gamma'}. \tag{11}$$

Hence, utilizing the expressions (3), (8a), (9), we shall obtain the T-matrix :

$$T_{\Gamma\Gamma_0} = \delta_{\Gamma\Gamma_0} e^{i\eta_0}\sin\eta_0 - \frac{1}{k}\int_0^\infty \bar{F}_\Gamma \sum_{\Gamma'} U_{\Gamma\Gamma'}\bar{F}_{\Gamma'}\, dr. \tag{12}$$

2. POLARIZATION POTENTIAL. REPRESENTATION OF DISTORTED WAVES.

Let us now make use of consecutive approximation method for the solution of the system of integral equations (11), taking for initial : $F_\Gamma^{(0)} = \bar{F}_{\Gamma_0}\delta_{\Gamma\Gamma_0}$. We shall have in the first approximation :

$$F_{\Gamma_0}^{(1)} = \bar{F}_{\Gamma_0}; \quad F_\Gamma^{(1)} = \hat{G}_\Gamma U_{\Gamma\Gamma_0}\bar{F}_{\Gamma_0}, \qquad (13)$$

$$(\Gamma \neq \Gamma_0)$$

$$T_{\Gamma_0\Gamma_0}^{(1)} = e^{i\eta_0}\sin\eta_0; \quad T_{\Gamma\Gamma_0}^{(1)} = -\frac{1}{k}\int_0^\infty \bar{F}_\Gamma U_{\Gamma\Gamma_0}\bar{F}_{\Gamma_0}dr. \qquad (14)$$

This is the known first approximation of the distorted wave method. The functions $\bar{F}_\Gamma$ are wave functions of elastic scattering in the Hartree-Fock approximation (i.e. in a stationary field U_Γ without accounting the atom polarization by the outer electron). If we replace L_Γ by a free motion operator (i.e. if we drop all U_Γ), we shall obtain the first Born approximation in the representation of partial waves. At the same time all $\eta = 0$ and

$$\bar{F} = krj_\ell(kr); \quad \bar{\bar{F}} = irh_\ell^{(1)}(kr) \quad (k^2>0), \qquad (15a)$$

$$\bar{F} = qri_\ell(qr); \quad \bar{\bar{F}} = rk_\ell(qr) \quad (k^2<0), \qquad (15b)$$

where j_ℓ and $h_\ell^{(1)}$ are Bessel and Hankel spherical functions, and i_ℓ and k_ℓ are the corresponding functions of the fictitious argument.

Effecting the following iterations and pursuing the process to as high as desirable approximations, we obtain the exact solution in the form :

$$F_\Gamma = F_\Gamma^{(1)} + \hat{G}_\Gamma V_{\Gamma\Gamma_0}\bar{F}_{\Gamma_0}. \qquad (16)$$

$$T_{\Gamma\Gamma_0} = T_{\Gamma\Gamma_0}^{(1)} - \frac{1}{k}\int_0^\infty \bar{F}_\Gamma V_{\Gamma\Gamma_0}\bar{F}_{\Gamma_0}dr. \qquad (17)$$

The correction for the elastic ($\Gamma = \Gamma_0$) and inelastic ($\Gamma \neq \Gamma_0$) scattering has an identical form. $\hat{G}_\Gamma V_{\Gamma\Gamma_0}$ is the resolvent of the system (11).

The sense of $V_{\Gamma\Gamma_0}$ is particularly clearly seen from the expression for the amplitude of the inelastic scattering:

$$T_{\Gamma\Gamma_e} = -\frac{1}{k}\int_0^\infty \bar{F}_\Gamma(U_{\Gamma\Gamma_e}+V_{\Gamma\Gamma_e})\bar{F}_{\Gamma_e}\,dr. \qquad (18)$$

As may be seen, $V_{\Gamma\Gamma_0}$ describes the correction for the mean potential at the expense of the correlation of electron motion (flow). That is why $V_{\Gamma\Gamma_0}$ may be called the polarization potential (generalized). The nonlocal character constitutes its essential peculiarity:

$$V_{\Gamma\Gamma_e}\varphi = \int_0^\infty V_{\Gamma\Gamma_e}(r,\ r')\varphi(r')\,dr'. \qquad (19)$$

$V_{\Gamma\Gamma_0}$ may be represented in the form of series by powers $U_{\Gamma_i\Gamma_k}$:

$$V_{\Gamma\Gamma_e} = \sum_a \sideset{}{'}\sum_{\Gamma_{1\cdots}\Gamma_{a-1}} U_{\Gamma\Gamma_1\ldots\Gamma_{a-1}\Gamma_e} \qquad (20)$$

$$U_{\Gamma\Gamma_1\ldots\Gamma_{a-1}\Gamma_e} = U_{\Gamma\Gamma_1}\hat{G}_{\Gamma_1}U_{\Gamma_1\Gamma_2}\ldots\hat{G}_{\Gamma_{a-1}}U_{\Gamma_{a-1}\Gamma_e}. \qquad (21)$$

The kernel of the operator $U_{\Gamma\Gamma_1\ldots\ldots\ldots\Gamma_{a-1}\Gamma_e}$ obviously has the form:

$$U_{\Gamma\Gamma_1\ldots\Gamma_{a-1}\Gamma_e}(r,\ r') =$$
$$=\int dr_1\ldots dr_{n-2}\,U_{\Gamma\Gamma_1}(r)\,G_{\Gamma_1}(r,\ r_1)\ldots U_{\Gamma_{a-1}\Gamma_e}(r'). \qquad (21a)$$

Let us finally note still another essential circumstance. According to the expression (8a), the functions $\bar{F}$ are complex. Let us introduce the real function $\bar{F}=e^{i\eta}F'$. Then the matrix element of the elastic collision will be written in the form

$$T_{\Gamma_0\Gamma_0}=e^{i\eta_0}\left\{\sin\eta_0 - \frac{e^{i\eta_0}}{k_0}\int_0^\infty F'_{\Gamma_0}V_{\Gamma_0\Gamma}F'_{\Gamma_0}\,dr\right\}. \qquad (18a)$$

The integral in the right-hand part is real, and, as a rule, negative (at least in the adiabatic approximation). That is why the polarizational correction is somehow shifted in phase by a quantity η_0 relative to the first approximation. Formula (18) attests to the fact that such shift is absent for the inelastic scattering.

3. REPRESENTATION OF THE ELASTIC SCATTERING

In the above-presented formulas the polarization was factually taken into account within the framework of the perturbation theory. Let us consider now another representation in which exact wave functions of elastic scattering $\mathcal{F}_\Gamma$ are utilized in an arbitrary state Γ. Such a function constitutes the solution of the Schrödinger one-part equation :

$$[L_\Gamma = \mathcal{V}_\Gamma + k^2]\, \mathcal{F}_\Gamma = 0,\qquad (22)$$

$$\mathcal{F}_\Gamma \sim e^{i\delta}\sin\left(kr - \frac{l\pi}{2} + \delta\right) = \sin\left(kr - \frac{l\pi}{2}\right) +$$

$$+ T_{\Gamma\Gamma} e^{i\left(kr - \frac{l\pi}{2}\right)},\quad \mathcal{F}_\Gamma(0) = 0,\qquad (23)$$

where δ is the exact phase of scattering and $\mathcal{V}_\Gamma$ is the new polarization potential. To determine it, we shall take advantage of the fact that, according to the expressions (13) and (16), $\mathcal{F}_\Gamma$ may be represented in the form

$$\mathcal{F}_\Gamma = \bar{F}_\Gamma + \hat{G}_\Gamma V_{\Gamma\Gamma}\mathcal{F}_\Gamma.\qquad (24)$$

On the other hand, the equation (22) may be rewritten in the form of integral equation

$$\mathcal{F}_\Gamma = \bar{F}_\Gamma + \hat{G}_\Gamma \mathcal{V}_\Gamma \mathcal{F}_\Gamma.\qquad (25)$$

Juxtaposing the equations (24) and (25), we obtain the equation for $\mathcal{V}_\Gamma$:

$$\mathcal{V}_\Gamma = V_{\Gamma\Gamma} - \mathcal{V}_\Gamma \hat{G}_\Gamma V_{\Gamma\Gamma},\qquad (26)$$

whence, equating the terms of identical order, we find

$$\mathcal{V}_\Gamma = \sum_n \sum_{\substack{\Gamma_1\ldots\Gamma_{n-1}\\ \Gamma_2\neq\Gamma}}' U_{\Gamma\Gamma_1\ldots\Gamma_{n-1}\Gamma},\qquad (27)$$

where the stroke at the sum points, as above, to the absence of terms including the diagonal potentials $U_{\Gamma_i\Gamma_k}$. The additional condition

notably diminishes the number of terms in the sum. The expression (27) is valid for any Γ, including $\Gamma = \Gamma_0$.

We shall pass now to the inelastic scattering. Its amplitude may be written by three equivalent methods :

$$T_{\Gamma\Gamma_0} = -\frac{1}{k} \int_0^\infty \bar{F}_\Gamma (U_{\Gamma\Gamma_0} - \mathcal{V}_{\Gamma\Gamma_0}^0) \mathcal{J}_{\Gamma_0} dr, \qquad (28a)$$

$$T_{\Gamma\Gamma_0} = -\frac{1}{k} \int_0^\infty \mathcal{J}_\Gamma (U_{\Gamma\Gamma_0} + \mathcal{V}_{\Gamma\Gamma_0}) \bar{F}_{\Gamma_0} dr, \qquad (286)$$

$$T_{\Gamma\Gamma_0} = -\frac{1}{k} \int_0^\infty \mathcal{J}_\Gamma (U_{\Gamma\Gamma_0} + \mathcal{V}_{\Gamma\Gamma_0}) \mathcal{J}_{\Gamma_0} dr. \qquad (28s)$$

Obviously, this corresponds to "initial", "final" and "symmetric" inclusion of polarization. The three expressions (28) are equivalent only in the case of exact solution of the problem. When using approximate functions $\mathcal{J}$ or potentials $\mathcal{V}$, these formulae lead to different results. Let us note that an analogus situation occurs in regard of exchange interaction (known "post" and "prior" approximations).

The connection of potentials $\mathcal{V}_{\Gamma\Gamma_0}$ and $V_{\Gamma\Gamma_0}$ is obtained by a method analogus to that utilizied when deriving the expression (26), but the computations are somewhat more cumbersome. We obtain as a result the following equations :

$$\mathcal{V}_{\Gamma\Gamma_0}^0 = V_{\Gamma\Gamma_0} - (U_{\Gamma\Gamma_0} + \mathcal{V}_{\Gamma\Gamma_0}^0) \hat{G}_{\Gamma_0} V_{\Gamma_0\Gamma_0};$$

$$\mathcal{V}_{\Gamma\Gamma_0} = V_{\Gamma\Gamma_0} - V_{\Gamma\Gamma} \hat{G}_\Gamma (U_{\Gamma\Gamma_0} + \mathcal{V}_{\Gamma\Gamma_0}); \qquad (29)$$

$$\mathcal{V}_{\Gamma\Gamma_0} = V_{\Gamma\Gamma_0} - (U_{\Gamma\Gamma_0} + \mathcal{V}_{\Gamma\Gamma_0}) G_{\Gamma_0} \mathcal{V}_{\Gamma_0\Gamma_0} -$$
$$- V_{\Gamma\Gamma} \hat{G}_\Gamma (U_{\Gamma\Gamma_0} + \mathcal{V}_{\Gamma\Gamma_0}) - V_{\Gamma\Gamma} \hat{G}_\Gamma (U_{\Gamma\Gamma_0} + \mathcal{V}_{\Gamma\Gamma_0}) G_{\Gamma_0} V_{\Gamma_0\Gamma_0}.$$

Substituting here the expansion by powers $U_{\Gamma_1\Gamma_k}$ we find

$$\mathcal{V}_{\Gamma\Gamma_0}^0 = \sum_n \sum_{\substack{i_1 \dots \\ \Gamma_{n-1}}} U_{\Gamma\Gamma_1} \dots \Gamma_{n-1}\Gamma_0; \qquad \mathcal{V}_{\Gamma\Gamma_0} = \sum_n \sum_{\substack{i_1 \dots \Gamma_{n-1}}} U_{\Gamma\Gamma_1} \dots \Gamma_{n-1}\Gamma_0;$$

$$\Gamma_i \neq \Gamma_0 \qquad\qquad\qquad \Gamma_i \neq \Gamma \qquad (30)$$

$$\mathcal{V}_{\Gamma\Gamma_0} = \sum_{n}\sum_{\Gamma_1\ldots\Gamma_{n-1}} U_{\Gamma\Gamma_1}\ldots\Gamma_{n-1}\Gamma_0 - \Delta\mathcal{V}_{\Gamma\Gamma_0}.$$

$$\Gamma_i\neq\Gamma, \ \Gamma_0$$

For $\Delta\mathcal{V}$ we shall limit ourselves to the expression till the 4th order :

$$\Delta\mathcal{V}_{\Gamma\Gamma_0} = U_{\Gamma\Gamma_0\Gamma\Gamma_0} + \sum_{\Gamma_1}[U_{\Gamma\Gamma_1\Gamma_0\Gamma\Gamma_0} + U_{\Gamma\Gamma_0\Gamma_1\Gamma\Gamma_0} + U_{\Gamma\Gamma_0\Gamma\Gamma_1\Gamma_0}]. \qquad (31)$$

Let us note that the nondiagonal potentials $\mathcal{V}$ and V coincide in the 2nd order, and the diagonal ones — to the 3rd order. We shall call the potentials $\mathcal{V}$ as well as V polarization potentials.

The representation of the exact problem of elastic scattering in the form of a three-dimensional one-part Schrodinger equation was made in the work [6] in a more abstract form. There too were formulated variational methods for the determination of $\mathcal{V}_\Gamma$. Certain partial expressions for the polarization potential of the 2nd order were given in Temkin works [3 — 5]. A nondiagonal polarization potential was also introduced in the work [9], but in a form somewhat different from the one utilized above.

4. APPROXIMATION OF TWO STATES

To illustrate the various representations it is useful to consider a two-level system. In the representation of the distorted waves $\bar{F}$ the transition amplitude will be written in the form:

$$T_{10} = -\frac{1}{k_1}\int_0^\infty \bar{F}_1(U_{10}+V_{10})\bar{F}_0\,dr. \qquad (32)$$

where V_{10} is the sum of terms of odd order :

$$V_{10} = U_{10}\hat{G}_0 U_{01} G_1 U_{10} + \ldots \qquad (33)$$

At the same time, in nonsymmetrical representations of elastically-scattered waves $\mathcal{V}_{10}{}^0 = \mathcal{V}_{10}{}^1 = 0$, т. е.

$$T_{10} = -\frac{1}{k_1}\int_0^\infty \bar{F}_1 U_{10}\mathcal{F}_0\,dr = -\frac{1}{k}\int_0^\infty \mathcal{F}_{-1}U_{10}\bar{F}_0\,dr. \qquad (34)$$

At the same time the polarization is fully accounted for in the functions F. Moreover, in diagonal potentials only the terms of the 2nd order are different from zero:

$$\mathcal{V}_0 = U_{01}\hat{G}_1 U_{10}; \quad \mathcal{V}_1 = U_{10}\hat{G}_0 U_{01}. \tag{35}$$

A symmetrical representation of the expression (28a) in case of a two-level problem is less practical, for it leads to overestimation of the polarization in wave functions ensuing $\mathcal{V}_{10} \neq 0$, and namely :

$$\mathcal{V}_{10} = -V_{10}.$$

It must however be underlined that a similar result refers only to a two-level approximation. In the presence of virtual levels the symmetrical representation may result very useful.

The representation of elastic scattering permits the subdivision of trajectory distortion effects and — specifically — the transitions to be made in a more evident fashion. Generally speaking, the introduction of but only an approximate expression for $\mathcal{V}_\Gamma$ into the equation for elastic scattering is usually more appropriate than the utilization of the perturbation theory with the very same approximate expression for $V_{\Gamma\Gamma}$.

Thus, thanks to the introduction of the polarization potential the solution of a type (2) - or (11)— infinite system is replaced by the solution of independent equations (6) for $\overline{F}$ and $\overline{\overline{F}}$, and also (in the second representation) of equations (22). Naturally, in their general form these transformations bear a formal character, since the difficulty of the solution of an infinite system are transfered to the computation of a complex series. However, the physical sense of the equations with a polarization potential appears to be significantly more descriptive. Besides, the formulation of approximate methods for the potential is in many case simpler and more descriptive than for wave functions.

II. APPROXIMATE REPRESENTATIONS OF THE POLARIZATION POTENTIAL.

1. Approximation of the 2nd Order.

In this subdivision we shall limit ourselves to the approxima-
tion of the 2nd order (i.e. to the first disappearing approximation)
for the polarization potential. At the same time, as was shown above,
the expressions for V, $\mathcal{V}^0$, $\mathcal{V}^1$ and $\mathcal{V}$ coincide. For the sake of defi-
niteness, we shall write in the following $\mathcal{V}_{\Gamma\Gamma_0}$, while the formulas
brought up will be in an equal measure valid for a diagonal potential
(at $\Gamma = \Gamma_0$).

Preserving only the term of 2nd order, $\mathcal{V}_{\Gamma\Gamma_0}$ may be written in
the form of a sum by a single set of intermediate distances $(a_1 \tilde{l}_1)$:

$$\mathcal{V}_{\Gamma\Gamma_0} = \sum_{a_1 \tilde{l}_1} U_{\Gamma\Gamma_1\Gamma_0} = \sum_{a_1 \tilde{l}_1}' U_{\Gamma\Gamma_1} \hat{G}_{\Gamma_1} U_{\Gamma_1\Gamma_0}. \qquad (36)$$

Here a_1 is a set of atom quantum numbers, $\tilde{l}_1$ is the orbital quantum
number of the outer electron. The quantum numbers L_T, S_T, k_1 are deter-
mined by the law of energy and moment preservation, and thus do not
enter into the number of summation indices. In particular,

$$k_1^2 = k_0^2 + \varepsilon_0 - \varepsilon_1 = k^2 + \varepsilon - \varepsilon_1, \qquad (37)$$

where ε_0 and ε_1 are the energies of the initial and intermediate
states of the atom.

Formula (36) may be written somewhat differently, taking
advantage of the spectral representation of the Green functions :

$$G_{\Gamma_1}(r, r') = \sum_{k_1'} \frac{F_{k_1'}(r) F_{k_1'}(r')}{k_1'^2 - k_1^2}, \qquad (38)$$

where the summation spreads over all the operator's L_{Γ_1} eigenvalues
(including the continuous spectrum; see formulae (4) and (7)). Substi-
tuting the equalities (37) and (38) into the formula (36), we obtain

../..

$$\mathcal{V}_{\Gamma\Gamma_0}(r,r') = \sum_{a_1 l_1 \, k_1} \frac{U_{\Gamma\Gamma_1}(r) F_{k_1'}(r) F_{k_1'}(r') U_{\Gamma_1\Gamma_0}(r')}{\varepsilon_1 + k_1'^2 - \varepsilon_0 - k_0^2}. \qquad (39)$$

The expression for $\mathcal{V}_{\Gamma\Gamma_0}$ by radial integrals is brought up in Addendum 2.

2. ADIABATIC APPROXIMATION.

In a greater part of practical calculations the so-called adiabatic approximation is being utilized. It may be obtained by assuming the Green function in intermediate state equal to

$$G_{\Gamma_1}(r, r') = -\frac{1}{\Delta\varepsilon}\delta(r-r'). \qquad (40)$$

This expression follows outright from the spectral representation of the expression (38), if we take advantage of the completeness of functions' F_{k_1}' assembly, assuming then $k_1'^2 - k_0^2 \ll \varepsilon_1 - \varepsilon_0$. Obviously, we may take for $\Delta\varepsilon$, with equal success, $\Delta\varepsilon = \varepsilon_1 - \varepsilon_0$ and $\Delta\varepsilon = \varepsilon_1 - \varepsilon$.

In the adiabatic approximation the "nonlocality" of the polarization potential is only connected with the exchange effects (see Addendum 2). Let us pause at further length on the most important particular case — diagonal polarization potential without accounting the exchange. According to formula (36) and (P. II), we then have

$$\mathcal{V}_\Gamma(r) = -\sum_{\varkappa\varkappa'}\sum_{a_1}{}' \frac{a_{\Gamma\Gamma_1}^\varkappa a_{\Gamma_1\Gamma}^{\varkappa'}}{\varepsilon_1 - \varepsilon} y_{aa_1}^\varkappa(r)\, y_{a_1a}^{\varkappa'}(r). \qquad (41)$$

For greater clarity of the following here and further, radial integrals are denoted $y_{aa_1}^\varkappa$ instead of $y_{ll_1}^{\varkappa'}$ which also underlines that radial functions of the optical electron factually depend on all the quantum numbers of the atom.

The potential $\mathcal{V}_\Gamma$ in (41) depends on the quantum numbers of the outer electron $\tilde{l}_1$ and $\tilde{l}$ and on the total moment L_T. If we substitute it by the expression averaged by L_T, the summing up by $\tilde{l}_1$ may be clearly fulfilled utilizing formulae from the Addendum 1 .

As a result we obtain $(a=L_p S_p n_1 l_1 L_1, \ L_p S_p$ being the moments of the initial ion):

$$\mathcal{Q}_\kappa^z(r) = \mathcal{Q}_a(r) = -\sum_\kappa \sum_{n_1 l_1 L_1}' \frac{4 Q_{aa_1}^\kappa}{(2\kappa+1)(2L+1)(\varepsilon_1 - \varepsilon)} [y_{aa_1}^\kappa(r)]^2, \quad (42)$$

$$a_1 \neq a$$

where $Q_{aa_1}^\kappa$ is the part of the expression for the oscillator of the $2\kappa-$ pole transition depending upon the moments; in the general case it may be written using 6j and 3j - symbols:

$$Q_{aa_1}^\kappa = (2S+1)(2L+1)(2L_1+1)\left\{\begin{matrix} l L L_p \\ L_1 P_1 \kappa \end{matrix}\right\}^2 (2l+1)(2l_1+1)\left(\begin{matrix} l l_1 \kappa \\ 0 0 0 \end{matrix}\right)^2. \quad (43)$$

The summation by n_1 in the equality (42) may be replaced by the solution of an auxiliary equation with the aid of a well-known procedure (see for example the owrk in ref. [6]). Assume that the functions $P_{a_1}(r)$ are the solutions of the Hartree-Fock equation

$$[L_{a_1} - \varepsilon_1] P_{a_1} = 0, \quad (44)$$

and that the function $\varphi(r', r)$ is the solution of the inhomogenous equation

$$[L_{a_1} + \varepsilon_1] \varphi(r', r) = -K_1^\kappa(r', r) P_a(r'), \quad (45)$$

$$K_1^\kappa(r', r) = \frac{r_<^\kappa}{r_>^{\kappa+1}} - \delta_{l_1 l} \int_0^\infty \frac{r_<^\kappa}{r_>^{\kappa+1}} P_a^2(r') \, dr'. \quad (46)$$

(here the operator L_{a_1} acts on the coordinate r'):

The substitution $\varphi(r', r) = g(r', r) P_a(r')$ is easy to effect in the equation (45). The function g satisfies the equation

$$g'' + 2 \frac{P_a'}{P_a} g' + \Delta L g = -K_1^\kappa(r', r) \quad (47)$$

(the derivatives in the left-hand part are taken by r'). The operator $\Delta L = L_{a_1} - L_a$ has a very simple form in cases offering interest.

As is well knownm the Hartree-Fock operator L_{a_1} depends on the main quantum number n_1 only through the nondiagonal parameters $\varepsilon_{n_1 n}$. Inasmuch as we do not take everywhere the nonorthoganility of atomic radial functions into account, this dependence can be neglected. Then, utilizing a method analogus to that used in the work [6], we may show that

$$\sum_{m} \frac{1}{\varepsilon_1 - \varepsilon} [y^{x}_{a a_1}(r)]^2 = \int_0^{\infty} K_1^{x}(r', r) \varphi(r', r) P_a(r') \, dr' =$$

$$= \int_0^{\infty} K_1^{x}(r', r) g(r', r) P_a^2(r') \, dr' \qquad (48)$$

and, consequently,

$$\mathcal{V}_a(r) = - \sum_{x L_1} \frac{4 Q^{x}_{a a_1}}{(2x+1)(2L+1)} \int_0^{\infty} K_1^{x}(r', r) g(r', r) P_a^2(r') \, dr'. \qquad (49)$$

The function g depends on the states a and a_1. If we neglect the weak dependence of g on L_1, and if we effect the summation by L_1, we shall obtain

$$\mathcal{V}_a(r) = - \sum_{x l_1} \frac{4(2l_1+1)}{2x+1} \begin{pmatrix} l & l_1 & x \\ 0 & 0 & 0 \end{pmatrix}^2 \int_0^{\infty} K_1^{x}(r', r) g(r', r) P_a^2(r') \, dr'. \qquad (49a)$$

At $\Delta L = 0$ (to that effect it is generally speaking necessary that $l_1 = l$; $L_1 = L$.) the equation (48) is resolved in quadratures:

$$g(r', r) = \int_0^{r} \frac{dx}{P_a^2(x)} \int_x^{\infty} K_1^{x}(x_1, r) P_a^2(x_1) \, dx_1. \qquad (50)$$

Let us examine now the behavior of $\mathcal{V}_r(r)$ at $r \to 0$ and $r \to \infty$. In the first case $y_x(r) \sim r^x$ and the basic role is played by the term with $x = 0$, i.e. with $l_1 = l$ and $L_1 = L$. Formula (49) gives

$$\mathcal{V}_a(0) = -4 \int_0^\infty \frac{dr}{P_a^2(r)} \left[\int_r^\infty \left(\frac{1}{x} - \left\langle \frac{1}{x} \right\rangle \right) P_a^2(x)\, dx \right];$$

(51)

$$\left\langle \frac{1}{x} \right\rangle = \int_0^\infty \frac{1}{x} P_a^2(x)\, dx.$$

In order to estimate this quantity we shall postulate
(A being the normalizing factor). Then, we have for the neutral
atom $\mathcal{V}_a(0) = -1/\mu^2 = \left\langle \frac{1}{r} \right\rangle$.

At $r \to \infty$ the term with $\varkappa = 0$ in $\mathcal{V}_a$ decreases exponen-
tially. At $\varkappa \neq 0$, $y^\varkappa \sim r^{-\varkappa-1}$ and the main role is played by the
term with $\varkappa = 1$, i.e. with $l_1 = l \pm 1$. From the expression (42) we
obtain the well known expression:

$$\mathcal{V}_a(r) \underset{r \to \infty}{\sim} -\frac{b}{r^4}; \quad b = \sum_{a_1} \frac{4 f_{aa_1}}{(\varepsilon_1 - \varepsilon)^2},$$

(52)

where b is the atom polarizability, and f_{aa_1} is the force of the dipole
transition oscillator.

It must be noted that although the dependence $\mathcal{V}_a \sim r^{-4}$ $(r \to \infty)$
is general, the expression for the coefficient b is only valid after
averaging $\mathcal{V}_a$ by L_T.

In practical calculations the approximate expression of the form

$$\mathcal{V}_a(r) = -\frac{b}{(r_0^2 + r^2)^2},$$

(53)

where $r_0 = \langle r \rangle$, i.e. is equal to mean radius for the optical elec-
tron, is often utilized. This formula gives a correct asymptotic for
$\mathcal{V}_a(r)$, but at $r = 0$, $\mathcal{V}_a = -b/r_0^4$. For hydrogen this quantity is
equal to -0.8, while the correct value is equal to -1. The error
becomes significantly greater if for the main term in the sum (52)
$-\varepsilon_1$, $-\varepsilon \ll \varepsilon$. Thus, for Na, $b/r_0^4 = 1.1$, while a most correct estimate
gives $|\mathcal{V}_a(0)| = 0.4$. Generally, formula (53) apparently gives in most
cases an overrated value for $|\mathcal{V}_a(0)|$. In connection with that it
should be noted, that the accounting of nonadiabaticity leads, as will
be shown below, to the value $\mathcal{V}_a(0) = 0$.

3. DISRUPTION OF ADIABATICITY

In the adaiabatic approximation the Green function of the
compound state is assumed proportional to the δ — function (formu-
la (40). In reality, this function has a finite width, which leads
to the "nonlocality" of the polarization potential and may, general-
ly speaking, substantially reflect upon the results. For the qualita-
tive clarification of the role of this effect we may utilize for G_{r_1}
the Born approximation with $l_1 = 0$.

According to formula (15), we then have for the energetically
unattainable intermediate states

$$G_{r_1} \approx G_{q_1} = -\frac{1}{2q_1} [e^{-q_1|r-r'|} - e^{-q_1|r+r'|}] \quad (k_1{}^2 < 0), \qquad (54)$$

$$q_1{}^2 = -k_1{}^2 = \varepsilon_1 - \varepsilon_0 - k_0{}^2 = \varepsilon_1 - \varepsilon - k^2, \qquad (55)$$

and for energetically attainable intermediate states

$$G_{r_1} \approx G_{k_1} = -\frac{1}{2ik_1} [e^{ik_1|r-r'|} - e^{ik_1|r+r'|}] \quad (k_1{}^2 > 0). \qquad (56)$$

It must be stressed that the utilization of the functions G_{q_1} or G_{k_1}
instead of the exact function G_r has only a slight smoothing
effect on polarization potential's kernel "smearing out", without
influencing the character of interaction. It may therefore be expect-
ed that such an approximation will be applicable also for real quan-
titative calculations.

Let us consider again the case of diagonal polarization poten-
tial without the exchange terms, assuming at the same time the energy
of the outer electron to be so low that $k_1^2 < 0$ for all intermediate
levels. The adiabatic approximation is generally applied precisely
in this region. Its ineffectiveness at high energies becomes obvious.
Inasmuch as G_{q_1} does not depend on $\tilde{l}_1$, we may again effect the ave-
raging by L_T. Then, instead of the expression (42) we shall obtain

the nonlocal operator with a kernel

$$\mathcal{V}_a(r, r') = \sum_{\varkappa \neq a} \sum \frac{4Q^\varkappa}{(2\varkappa+1)(2L+1)} y^\varkappa_{\mu_1}(r) G_{q_1}(r, r') y^\varkappa_{\mu'}(r'). \quad (57)$$

Fig.1 shows $G_{q_1}(r, r')$ at $r = 1$ and two values of q. It must be noted first of all that

$$-\int \Delta \varepsilon G_{q_1} dr' = \frac{\Delta\varepsilon}{q_1^2}(1-e^{-\varepsilon_1 r}) \quad (\Delta\varepsilon = \varepsilon_1 - \varepsilon),\qquad (58)$$

while in the adiabatic approximation the left-hand part of the expression (58) is equal to the unity. For not too small values of q_r $\left(q_1^2 \gtrsim \frac{\Delta\varepsilon}{2}\right)$, when the width of
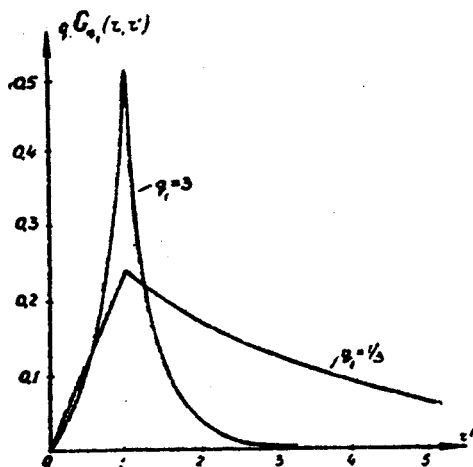

FIG.1

the function G_{q_1} still is rather small, we may utilize as a first correction the adiabatic potential, multiplied by the factor (58). Let us note that this factor is zero at $r = 0$ and it is greater than the unity at greater r, since $q_1^2 < \Delta\varepsilon$.

The width of G_{q_1} increases with the decrease of $q_1 (k^2 \to \Delta\varepsilon)$, and at $q_1 \to 0$ $G_{q_1} = \min\left\{r, r'\right\}$, i.e. it has nothing in common with the δ— function. In particular, the integral (58) diverges. If G_{q_1} varies more slowly than $y^\varkappa(r)$ and $\overline{F}_r(r)$, the transition to the local potential is generally impossible.

In the adiabatic approximation the polarizational correction for the elastic scattering is given by the linear combination of integrals of the type

$$\int [y^\varkappa(r)\overline{F}_r(r)]^2 dr.$$

In another boundary case $q_1 \to 0$ we have

$$\iint y^*(r)\bar{F}_\Gamma(r)y^*(r')\bar{F}_\Gamma(r')r_< \, dr\, dr'.$$

The oscillations of the subintegral function may play an important part in the last integral. We thus may expect a decrease of polarization effects by comparison with the adiabatic approximation. Whether or not this effect or the correction for the normalization (58) will predominate — it depends upon the concrete conditions.

Usually it is required as a condition of applicability of the adiabatic approximation that the velocity of the outer electron be much lower than that of the optical electron, i.e. $k^2 \ll \varepsilon$. Stiffer requirements stem from the above-conducted analysis :

1) $q_1^2 \approx \Delta\varepsilon$, i. e. $k^2 \ll \Delta\varepsilon < \varepsilon$;

2) $q_1 \gg \dfrac{1}{a}$

where a is the dimension of the region in which $y^x_{l l_1}(r)$ varies significantly. The value of q_1 depends on the energy of the intermediate state ε_1. That is why the conditions of adiabadicity may be fulfilled for some intermediate states, and not for the others. In fact however, it is usually possible to separate in the sum by a_1 in the formula (24) one main term, which simplifies very much the calculations.

The author expresses its deep appreciation to I. I. Sobel'man for discussing the present paper.

*** THE END ***

Addenda 1 and 2 follow..

APPENDIX

The expression for the potential $U_{\Gamma\Gamma'}$ includes the parameters $\lambda_{\Gamma\Gamma}, \alpha^{x}_{\Gamma\Gamma'}, \beta^{x}_{\Gamma\Gamma'}$. Presented below are the formulae for these parameters.

$$\lambda_{\Gamma\Gamma'} = -\varepsilon_{l'} + \frac{k^2}{2} = -\varepsilon_l + \frac{k'^2}{2},$$

where ε_l and $\varepsilon_{l'}$ are the energetic parameters of the Hartree-Fock equation for the optical electron. However, it should be noted that the equality if formula (Ad.1) takes place only approximately (with a precision to the variation of polarization energy of the atomic residuum at optical electron transition).

If

$$\Gamma = a\tilde{l}L_T S_T; \quad a = \gamma L_P S_P l \frac{1}{2} LS,$$

where $L_P S_P$ are the moments of the original ion, $l\,\tilde{l}$ are the moments of the optical and outer electrons, LS — the moments of the atom and $L_T S_T$ the total moments of the system, then

$$\alpha^{x}_{\Gamma\Gamma'} = \delta_{SS'} (-1)^{L_T + l + \tilde{l}'} (l\|C^x\|l')(\tilde{l}\|C^x\|\tilde{l}') \begin{Bmatrix} x L L' \\ L_T \tilde{l}' \tilde{l} \end{Bmatrix} \mu^{x}_{\Gamma\Gamma'};$$

$$\beta^{x}_{\Gamma\Gamma'} = (-1)^{S_T + \frac{1}{2} - S + l + \tilde{l}'} (l\|C\|\tilde{l}')(\tilde{l}\|C^x\|l') \begin{Bmatrix} x L \tilde{l}' \\ L_T L' \tilde{l} \end{Bmatrix} v^{x}_{\Gamma\Gamma'},$$

where
$$(l\|C^x\|l') = (-1)^l (2l+1)^{\frac{1}{2}} (2l'+1)^{\frac{1}{2}} \begin{Bmatrix} l\,l'\,x \\ 0\,0\,0 \end{Bmatrix}.$$

In case $L_P = S_P = 0$ (one electron beyond the filled shells) $\mu^{x}_{\Gamma\Gamma'} = v^{x}_{\Gamma\Gamma'} = 1$. In a more general case $\mu^{x}_{\Gamma\Gamma'} = \delta_{PP'} (-1)^{x+L+L'} (2L+1)^{\frac{1}{2}} (2L'+1)^{\frac{1}{2}} \begin{Bmatrix} x L L' \\ L_P \tilde{l}'\,l \end{Bmatrix};$

$$v^{x}_{\Gamma\Gamma'} = \delta_{PP'} (-1)^{S_T - \frac{1}{2} - S'} (2S+1)^{\frac{1}{2}} (2S'+1)^{\frac{1}{2}} \begin{Bmatrix} S_T \frac{1}{2} S \\ S_P \frac{1}{2} S \end{Bmatrix} \times$$

$$\times (2L+1)^{\frac{1}{2}} (2L'+1)^{\frac{1}{2}} \begin{Bmatrix} x L \tilde{l} \\ L_T L' \tilde{l} \end{Bmatrix}^{-1} \sum_{L_2} (2L_2+1) \begin{Bmatrix} \tilde{l} L L_2 \\ L_P L_T L \end{Bmatrix} \times \begin{Bmatrix} \tilde{l}' \tilde{l}' L_2 \\ L_P L_T L' \end{Bmatrix} \begin{Bmatrix} \tilde{l} l L_2 \\ \tilde{l}' l' x \end{Bmatrix}.$$

If the atom has in the state **a** **N** equivalent electrons and consequently, the term $L_p S_p$ is not given, then $\mu_{rr'}^x$ and $v_{rr'}^x$ ought to be averaged by $L_p S_p$, i.e. instead of (Ad. 4) α and β should be substituted into the mean values

$$\bar{\mu}_{rr'}^x = \sum_{L_p S_p} G^{LS}_{L_p S_p} \mu_{rr'}^x; \quad v_{rr'}^x = \sum_{L_p S_p} G^{LS}_{L_p S_p} v_{rr''}^x$$

where $G^{LS}_{L_p S_p}$ are the Racah genealogical coefficients. The averaging by $L_p S_p$, utilizing the coefficients $G^{L'S'}_{L_p S_p}$, must be effected in exactly the same way, provided there exist in the state a' several equivalent electrons in the outer shell.

We shall bring forth some particular values of the coefficients α and β. As may be seen from formulae (Ad. 3), (Ad. 4), α is not dependent on spin (if we do not consider the selection rule $S = S'$), while β may be written in the form of a product of independent multipliers :

$$\beta = \beta(S)\beta(L). \tag{Ad. 6}$$

At $S_p = 0$

$$S_r = 0; \ 1; \quad \beta(S) = (-1)^{s_r+1}. \tag{Ad. 7}$$

At $S_p = \frac{1}{2}$, three types of transitions are possible:

$$^1L - ^1L'; \quad S_r = \frac{1}{2}; \quad \beta(S) = 1, \tag{Ad. 8a}$$

$$^1L - ^3L'; \quad S_r = \frac{1}{2}; \quad \beta_{rr}(S) = \beta_{rr'}(S) = 1; \quad \beta_{r'r} = \frac{3}{2}, \tag{Ad. 8}$$

$$^3L - ^3L'; \quad S_r = \frac{1}{2}; \ \frac{3}{2}; \ \beta(S) = \frac{3\left(S_r + \frac{1}{2}\right)}{2}(-1)^{s_r+\frac{1}{2}}. \tag{Ad. 8}$$

Let us examine now the orbital part, limiting ourselves to the case $L_p = 0$. At the same time $L = $, $L' = l'$. The coefficients α^0_{rr} and $\alpha^0_{r'r'}$ are always equal to 1. Written velow are the coefficients different from zero. We utilize the denotation $g = 2\tilde{l} + 1$; $g' = 2\tilde{l}' + 1$.

1. The transition S — S : $l = l' = 0$; $\tilde{l} = \tilde{l}' - L_r$;

$$\alpha^0_{rr} = 1; \qquad\qquad \text{(Ad.9a)}$$

2. Transition S — P

$$\beta^{\tilde{l}}_{rr}(L) = \beta^{\tilde{l}}_{rr'}(L) = \beta^{\tilde{l}}_{r'r'}(L) = \frac{1}{g}.$$

$$l = 0; \quad l' = 1; \quad \tilde{l}' = \tilde{l} \pm 1; \quad L_r = \tilde{l};$$

$$\alpha^1_{rr} = \pm\left(\frac{g \pm 1}{6g}\right)^{\frac{1}{2}}; \quad \alpha^2_{r'r'} = \frac{g \pm 3}{10g};$$

$$\beta^{\tilde{l}}_{rr}(L) = \frac{1}{g}; \quad \beta^{\tilde{l}}_{rr'}(L) = \mp\frac{1}{g'}\left(\frac{3g \pm 1}{2g}\right)^{\frac{1}{2}};$$

$$\beta^{\tilde{l}}_{r'r'}(L) = \frac{3}{g'g^2}; \quad \beta^{\tilde{l}\pm 2'}_{r'r'}(L) = \frac{3(g \pm 3)}{2g'(g \pm 4)}.$$

<div style="text-align:right">ADDENDUM 2</div>

In the 2nd order of the perturbation theory, V_{rr_0} is expressed by the sum by Γ_1 from $U_{rr_1r_0}$:

$$U_{rr_1r_0}(r, r')\bar{F}_{r_0} = \sum_{\varkappa\varkappa'}\alpha^\varkappa_{rr_1}\alpha^{\varkappa'}_{r_1r_0}y^\varkappa_{ll_1}(r)\,G_{r_1}(r,r')\,y^{\varkappa'}_{l_1l_0}(r')\bar{F}_{r_0}(r') -$$

$$- \sum_{\varkappa\varkappa'}\alpha^\varkappa_{rr_1}\beta^{\varkappa'}_{r_1r_0}y^\varkappa_{ll_1}(r)\,G_{r_1}(r,r')\,y^{\varkappa'}_{l_1\tilde{l}_0}(r')\,P_{l_0}(r') -$$

$$- \sum_{\varkappa\varkappa'}\beta^\varkappa_{rr_1}\alpha^{\varkappa'}_{r_1r_0}P_{l_1}(r)\,y^\varkappa_{l0_1}(r,r')y^{\varkappa'}_{l_1l_0}(r')\bar{F}_{r_0}(r') + \qquad \text{(Ad.10)}$$

$$+ \sum_{\varkappa\varkappa'}\beta^\varkappa_{rr_1}\beta^{\varkappa'}_{r_1r_0}P_{l_1}(r)\,y^\varkappa_{l0_1}(r,r')\,y^{\varkappa'}_{l_1\tilde{l}_0}(r')\,P_{l_0}(r')$$

The radial integrals $y^\varkappa_{ll_1}$ and $y^\varkappa_{l\tilde{l}_1}$ are determined by the formulae (Add.5a) and (Ad.5); as to $y^\varkappa_{l0_1}$ it is obtained from the equality (5) by substituting $G_{\Gamma_1}(r, r')$ for $F_{\Gamma_1}(r_1)$. From the last determination it is evident that $y^\varkappa_{lG}$ is dependent upon two variables.

In the adiabatic approximation

$$G_{\Gamma_1} = -\frac{1}{\Delta \varepsilon} \delta(r - r')$$

and the integration over r' can be effected. The polarization potential (the first term of the right-hand part of formula (Ad.10)) becomes local, while the exchange terms preserve their nonlocality.
We obtain

$$U_{\Gamma\Gamma_1\Gamma_0}\bar{F}_{\Gamma_0} = \int_0^\infty U_{\Gamma\Gamma_1\Gamma_0}(r, r') \bar{F}_{\Gamma_0}(r') \, dr' =$$

$$= - \sum_{\varkappa\varkappa'} \frac{\alpha^\varkappa_{\Gamma\Gamma_1} \alpha^{\varkappa'}_{\Gamma_1\Gamma_0}}{\Delta\varepsilon} y^\varkappa_{ll_1} y^{\varkappa'}_{l_1 l_0} \bar{F}_{\Gamma_0} + \sum_{\varkappa\varkappa'} \frac{\alpha^\varkappa_{\Gamma\Gamma_1} \beta^{\varkappa'}_{\Gamma_1\Gamma_0}}{\Delta\varepsilon} y^\varkappa_{ll_1} y^{\varkappa'}_{l_1 \tilde{l_0}} P_{l_0} + \quad \text{(Ad.11)}$$

$$+ \sum_{\varkappa\varkappa'} \frac{\beta^\varkappa_{\Gamma\Gamma_1} \alpha^{\varkappa'}_{\Gamma_1\Gamma_0}}{\Delta\varepsilon} y^{\varkappa\varkappa'}_{l\tilde{l_0}l_1 l_0} P_{l_1} - \sum_{\varkappa\varkappa'} \frac{\beta^\varkappa_{\Gamma\Gamma_1} \alpha^{\varkappa'}_{\Gamma_1\Gamma_0}}{\Delta\varepsilon} y^{\varkappa\varkappa'}_{l_0 l_1 \tilde{l_0}} P_{l_0},$$

where the denotation

$$y^{\varkappa\varkappa'}_{l\tilde{l_0}l_1 l_0}(r) = 4 \int\int dr_1 \, dr_2 K^\varkappa(r, r_1) K^\varkappa(r, r_2) P_l(r_1) \bar{F}_{\Gamma_0}(r_1) P_{l_1}(r_2) P_{l_0}(r_2) \quad \text{(Ad.12)}$$

has been introduced, and $K^\varkappa$ are kernels of the integrals (5a) and (5b), while the form of the kernel must correspond in the respective term of (Ad.11) either to the coefficient $\varkappa$ or β.

END OF THE ADDENDA.

.. References ..

REFERENCES

[1]. L. VAYSHTEYN, I. SOBEL'MAN.- ZhETF, 39, 767, 1960.

[2]. B. BRANDSEN, A. DALGARNO, T. JOHN, M. SEATON. Proc. Phys. Soc.
                              71, 877, 1958.

[3]. A. TEMKIN.- Phys. Rev. 107, 1004, 1957.

[4]. A. TEMKIN.- Phys. Rev. 116, 358, 1959.

[5]. A. TEMKIN, J. LAMKIN.- Phys. Rev. 121, 788, 1961.

[6]. M. MITLLEMAN, K. WATSON.- Phys.Rev. 113, 198, 1959.

[7]. M. MITTLEMAN, K. WATSON.- Phys. Rev. 116, 920, 1959.

[8]. C. SCHWARTZ.- Ann. phys., 6, 156, 1959.

[9]. R. LIPPERHEIDE.- Ann.phys., 17, 114, 1962.

DISTRIBUTION

GODDARD SFC		NASA HQS.		OTHERS.
HESS	640	NEWELL, CLARK	SS	AMES
TEMKIN	641	STANSELL	SP	
		NAUGLE	SG	LANGLEY
MEREDITH	610	FELLOWS		LEWIS
MCDONALD	611	DUBIN		
KUPPERIAN	613	HIPSHER, HOROWITZ		MARSHALL
LINDSAY	614	PIEPER		JPL
BOURDEAU	615	LIDDEL	SL	AIAA
SPENCER	651	KURZWEG	RR	AID
WEAVER (LIB)	252	HARRISON	RRE	AIP
		WILSON	RRA	
		GESSOW	RRP	
		NEILL	RTR	
		SCHWIND	AFSS	